



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:30 AM GMT

PDB ID : 1J38
Title : Crystal Structure of Drosophila AnCE
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Deposited on : 2003-01-20
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

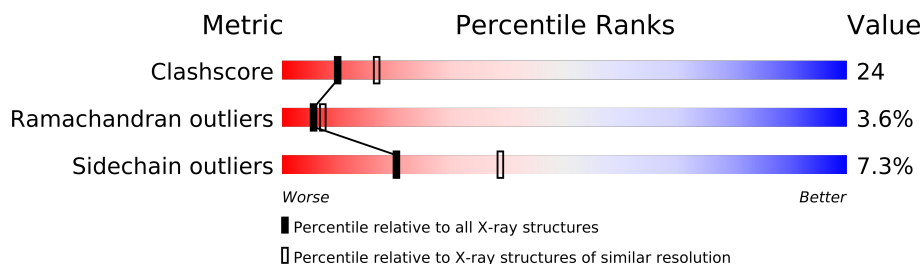
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	
1	B	607	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9806 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called angiotensin converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			
1	B	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	CONFLICT	UNP Q10714
A	53	ALA	ASN	CONFLICT	UNP Q10714
A	607	ILE	THR	CONFLICT	UNP Q10714
A	616	HIS	-	EXPRESSION TAG	UNP Q10714
A	617	HIS	-	EXPRESSION TAG	UNP Q10714
A	618	HIS	-	EXPRESSION TAG	UNP Q10714
A	619	HIS	-	EXPRESSION TAG	UNP Q10714
A	620	HIS	-	EXPRESSION TAG	UNP Q10714
B	51	ARG	GLY	CONFLICT	UNP Q10714
B	53	ALA	ASN	CONFLICT	UNP Q10714
B	607	ILE	THR	CONFLICT	UNP Q10714
B	616	HIS	-	EXPRESSION TAG	UNP Q10714
B	617	HIS	-	EXPRESSION TAG	UNP Q10714
B	618	HIS	-	EXPRESSION TAG	UNP Q10714
B	619	HIS	-	EXPRESSION TAG	UNP Q10714
B	620	HIS	-	EXPRESSION TAG	UNP Q10714

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	2	Total 2	O 2	0	0

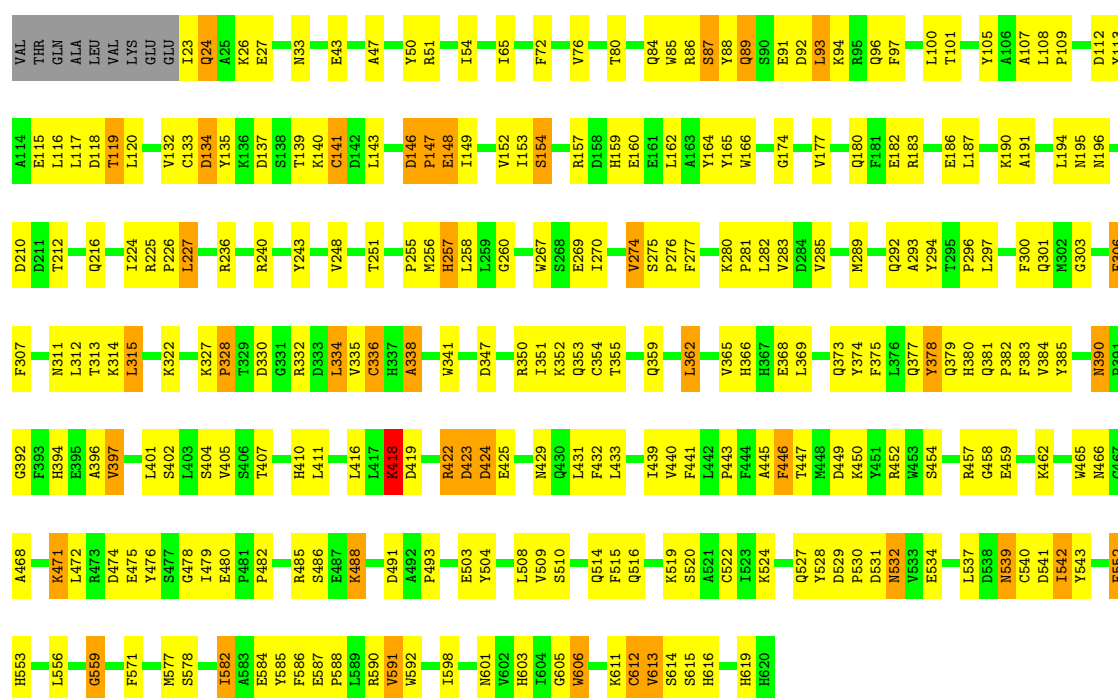
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

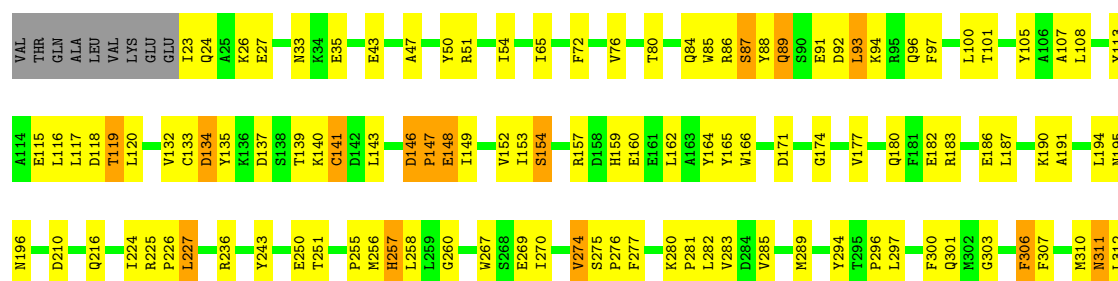
- Molecule 1: angiotensin converting enzyme

Chain A:



- Molecule 1: angiotensin converting enzyme

Chain B:



T313	V397	Y476	M577
K314	L401	S477	S578
L315	S402	G478	
		I479	
K322	V405	E480	I582
K327	S406	P481	A583
P328	T407	P482	E584
T329		R485	Y585
D330	H410	S486	F586
G331	L411	E487	E587
R332		P588	P588
D333	L416	K488	I589
L334	L417	D491	R590
V335	K418	A492	V591
C336	P493	P493	W592
H337	R422		
A338	D423	E503	N601
	D424	Y504	V602
W341	E425		H603
		L508	I604
D347	N429	V509	G605
	Q430	S510	W606
R350	L431		
I351	F432	Q514	N610
K352	L433	F515	K611
Q353		Q516	G612
C354	I439		V613
T355	V440	K519	S614
	F441	S520	S615
Q359	L442	A521	H616
	P443	C522	
L362	F444	I523	H619
	A445	K524	H620
V365	F446		
H366	T447	Q527	
H367	W448	Y528	
E368	D449	D529	
L369	K450	P530	
	Y451	D531	
Q373	R452	N532	
Y374	W453	W533	
F375	S454	E534	
L376			
Q377	R457	L537	
Y378	G458	D538	
Q379	E459	N539	
H380		C540	
Q381		D541	
P382	K462	I542	
F383	W465	Y543	
V384	N466	F552	
Y385	C467	H553	
	A468		
N390	K471	L556	
P391	L472		
G392	R473	G559	
F393	D474		
H394	E475	F571	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/5031	0.67	0/6814
1	B	0.45	0/5031	0.68	0/6814
All	All	0.44	0/10062	0.67	0/13628

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4900	0	4696	221	2
1	B	4900	0	4696	230	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	9806	0	9392	450	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

The worst 5 of 450 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ASP:HB3	1:A:147:PRO:HD3	1.39	1.04
1:B:146:ASP:HB3	1:B:147:PRO:HD3	1.39	1.01
1:A:143:LEU:HD22	1:A:148:GLU:HG2	1.42	1.00
1:B:143:LEU:HD22	1:B:148:GLU:HG2	1.46	0.96
1:B:347:ASP:H	1:B:379:GLN:HE22	0.95	0.94

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:619:HIS:NE2	1:B:134:ASP:OD2[1_554]	2.07	0.13
1:A:134:ASP:OD2	1:B:619:HIS:NE2[1_554]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/607 (98%)	517 (87%)	58 (10%)	21 (4%)	6	8
1	B	596/607 (98%)	518 (87%)	56 (9%)	22 (4%)	5	7
All	All	1192/1214 (98%)	1035 (87%)	114 (10%)	43 (4%)	5	7

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	147	PRO
1	A	418	LYS
1	A	542	ILE
1	B	24	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/530 (98%)	483 (92%)	39 (8%)	19	36
1	B	522/530 (98%)	485 (93%)	37 (7%)	21	40
All	All	1044/1060 (98%)	968 (93%)	76 (7%)	20	38

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	552	PHE
1	B	93	LEU
1	B	539	ASN
1	A	582	ILE
1	A	612	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	ASN
1	B	89	GLN
1	B	532	ASN
1	A	554	ASN
1	B	31	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.